

# 3-Methylcarbazole, n-trifluoroacetyl-

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | 3-Methylcarbazole, TFA                                                           |
| Inchi:               | InChI=1S/C15H10F3NO/c1-9-6-7-13-11(8-9)10-4-2-3-5-12(10)19(13)14(20)15(16,17)18/ |
| InchiKey:            | JSBGSIIQRBADII-UHFFFAOYSA-N                                                      |
| Formula:             | C15H10F3NO                                                                       |
| SMILES:              | <chem>Cc1ccc2c(c1)c1ccccc1n2C(=O)C(F)(F)F</chem>                                 |
| Mol. weight [g/mol]: | 277.24                                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| logp          | 4.305   |        | Crippen Method |
| mcvol         | 180.690 | ml/mol | McGowan Method |

## Sources

|                           |                                                                                                                                           |
|---------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U328378&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U328378&amp;Units=SI</a> |
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method:           | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |
| Cheméo Relay (1.0):       |                                                                                                                                           |
| Cheméo Relay (1.0, beta): |                                                                                                                                           |

## Legend

|        |                                     |
|--------|-------------------------------------|
| logp:  | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume     |

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